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16. ABSTRACT
The American Meteorological Society, under joint sponsorship from the U.S. Environmental Protection Agency, the Atmospheric Environment Service, Canada and the Ontario Ministry of the Environment, Canada, convened a workshop in September 1984 to address an aspect of long-range transport modeling that has become a topic of considerable concern, that is, the quantification of uncertainty in long-range transport model predictions and the implications of these uncertainties on formulations of control policy. A series of draft chapters provided a focus for discussion by 38 invited national and international experts in the areas of policy perspectives, methods for sensitivity and uncertainty analysis, and sources of errors and uncertainty in Eulerian, Lagrangian, and stochastic long-range transport models.

Composite uncertainty in model outputs consists of the meteorological, chemical, and emissions input data uncertainty combined with model formulation uncertainty, the latter due to representation of the physical-chemical processes and partly attributable to the mathematical integrations. Therefore, insight into a model's response to arbitrary varying inputs for a particular formulation is required in order to evaluate quantitative estimates of the expected change in air quality or deposition as a result of specific changes in emissions. This insight can then be put to use in determining the most effective strategies to mitigate air-pollutant-related environmental problems.

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SOURCES AND EVALUATION OF UNCERTAINTY IN LONG-RANGE TRANSPORT MODELS

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INTRODUCTION

A main concern in the areas of environmental protection, human health, resource management, and international relations is the quantitative determination of the relationships between the distribution and rate of pollutant emissions into the atmosphere, and the distribution, rate, and forms of surface deposition downwind. It needs also to be established that simulation models can be used with reasonable confidence to predict the air quality/deposition changes associated with emissions conditions different from those used to develop and test the models.

In addition to being responsive to the interests of policy analysts and resource managers, the simulation models and related evaluation programs must also be designed to meet the needs of effects researchers and air quality/deposition trends analysts. Their needs include determination of the spatial and temporal representativeness of point measurements made over specific time intervals in order to permit confident interpolation and extrapolation from limited observations of air quality and deposition. Information on the frequency of occurrence of extreme air quality/deposition events is also required for this purpose.

It should be recognized that user issues and priorities could reasonably change over time and that an important user-oriented guideline to the design of a model evaluation program is that it be robust and comprehensive. From a user perspective, it is equally important to know the uncertainties associated with predicted values as it is to insist that the model predictions are useful only if they are of certain precision. Therefore, conducting uncertainty analyses on the model predictions is a key user need, both in component and aggregate modes.

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Model uncertainty refers to the limits of variation in model predictions as a result of the approximate nature of the modeling system in precisely describing the meteorological and chemical processes occurring in the atmosphere, and of limits in our ability to precisely describe the state of the atmosphere via observational inputs to the model.

To empirically perform the model uncertainty analysis requires a rather extensive observational data set encompassing a broad range of meteorological and chemical conditions. Such data sets will allow the comparisons of model predictions and observations in order to generate probability distribution functions of differences between modeled and observed values. The difficulty with such comparisons is that some sources of uncertainty may not be resolvable. It may be possible through the selective partitioning of data sets to reduce some of the existing degrees of freedom and thus augment the resolution of the uncertainty analysis, but to date this has not yet been adequately demonstrated (Demerjian, 1985a).

During the past few years, however, various efforts have been directed to quantifying uncertainty in long-range transport models through comparative model evaluation exercises and by means of a recent international workshop. This paper will describe a sequence of events conducted through joint efforts of United States and Canadian scientists, concentrating on the conclusions reached during a workshop specifically designed to address the sources and evaluation of model uncertainty in long-range transport models.

MEMORANDUM OF INTENT

The Atmospheric Sciences and Analysis Work Group 2 was one of five work groups established under the Memorandum of Intent (MOI) on Transboundary Air Pollution, signed by the governments of Canada and the United States on August 5, 1980. The objectives of the work groups were to synthesize available knowledge about the causes and effects of transboundary air pollution, with the initial emphasis on acidic transport and deposition, for use by the governments of the two neighboring countries in negotiating a bilateral air quality agreement.

Under the auspices of Work Group 2, the Regional Modeling Subgroup conducted the evaluation of eight linear regional-scale sulfur transport models using standardized input and validation data sets. It was not possible to provide models for all of the pollutants of interest nor to incorporate all the processes mathematically into operational regional models. For example, deficiencies in both emissions inventories and in comprehension of transformation and deposition processes precluded the development of quantitative models for acid nitrate deposition. Nor was it possible to incorporate the detailed atmospheric chemical reactions between SO_2, NO_x, volatile organic compounds (VOC), oxidants, and their acidic reaction products. The models evaluated by Work Group 2, therefore, contained simplifying assumptions which were based upon our current understanding of the phenomena of long-range pollutant transport.

The Regional Modeling Subgroup attempted to compare the results from the selected models with network data in eastern North America for January, July, and annual 1978. However, the data from the networks were judged insufficient for conclusive model evaluation. The periods chosen, two sample months and one entire year, were too short, while the spatial distribution of the data was also poor. Air quality data were only available in the eastern United States while the precipitation chemistry data were mainly for Canada. Significant limitations also existed in the input emissions and precipitation data.

One of the original tasks for the Regional Modeling Subgroup was to recommend the best model(s) for future use in emission reduction scenarios. Towards this end, the input parameters of the models were displayed and model evaluation criteria were standardized to ascertain the model accuracies. However, due to uncertainties in the emissions inventory and in precipitation data used by the models as well as in the measurement data used for evaluation, even a ranking of models in terms of their absolute performance could not be made.

Furthermore, due to these deficiencies, it was not possible to quantify the uncertainties in model predictions based on the differences between model predictions and observations (residuals). As a result, the model evaluations only served as a demonstration of the statistical methodology to be used in such exercises and as a preliminary indication of model performance (Schiermeier and Misra, 1983).

AMS UNCERTAINTY WORKSHOP

As an outgrowth of the MOI effort, the quantification of uncertainty in long-range transport model predictions and the implications of these uncertainties on formulations of control policy remained topics of concern to representatives of both countries. To more fully address these topics, the American Meteorological Society (AMS) was requested to convene a workshop in September 1984 at the National Academy of Sciences Study Center in Woods Hole, Massachusetts. Joint sponsorship was provided by the U.S. Environmental Protection Agency, the Ontario Ministry of the Environment, Canada, and the Atmospheric Environment Service of Environment Canada.

Workshop Objectives

The AMS Workshop on Sources and Evaluation of Uncertainty in Long-Range Transport Models had these following objectives (American Meteorological Society, 1984):

- To examine our current understanding of the physical processes responsible for the long-range transport and deposition of atmospheric pollutants, with emphasis given to the uncertainties in our understanding of these processes;

- To examine the parameterization of these processes in available long-range transport models and to estimate the effects of these parameterizations on model uncertainty;

*To examine the temporal and spatial scales of applicability of the available long-range transport models;

*To examine the data base available for use in long-range transport modeling and, to the extent possible, estimate the limits of predictability associated with the use of this data base;

*To recommend methods to test long-range transport model results with corresponding observations with a view to quantifying model uncertainty;

*To produce a report summarizing the workshop findings.

Workshop Organization

The AMS workshop was three and one-half days in duration and involved participation by thirty-eight scientists from the United States, Canada, and Europe. Five invited draft chapters were prepared prior to the workshop to provide a focus for discussion, i.e., to raise the pertinent scientific issues to be addressed by the working groups and to aid in preparation of the findings and recommendations. The titles and authors of the five draft chapters were as follows:

"A Policy Perspective on Long-Range Transport Models" by Robert M. Friedman;

"Sources of Error and Uncertainty in Eulerian Long-Range Transport Models" by Gregory R. Carmichael;

"Sources of Uncertainty in Lagrangian Long-Range Transport Model Calculation" by Anton Eliassen;

"Stochastic Long-Range Transport Models" by Akula Venkatram;

"Methods for the Sensitivity and Uncertainty Analysis of Long-Range Transport Models" by Gregory J. McRae.

An AMS publication containing the complete documentation of the workshop including the revised chapters, recent developments in model evaluation and sensitivity analysis, and the reports of the Eulerian and Lagrangian working groups should be completed this spring (American Meteorological Society, 1987). This paper intends to provide a brief overview of the workshop recommendations on quantification of uncertainty in long-range model predictions and some implications of these uncertainties on formulations of control policy. Material will be drawn from the five invited chapters without specific attribution and from the published synopsis of the workshop (Demerjian, 1985b).

MODEL EVALUATION DATA

Composite uncertainty in model outputs includes the input data uncertainty combined with model formulation uncertainty, the latter due to our representation of the physical-chemical processes and partly attributable to the mathematical integra-

tions. The workshop participants were unanimous in indicating that the highest priority with regard to elucidation and quantification of uncertainty in long-range transport models is the development of improved data bases for model testing and performance evaluation. This is in keeping with the United States/Canada Modeling Subgroup conclusion that parts of the disagreement between the eight models' results were due to the different processing of the meteorological input data and the quality of that data (Schiermeier and Misra, 1982).

To empirically perform the model uncertainty analysis requires extensive observational data sets encompassing broad ranges of meteorological and chemical conditions. Such data sets will allow comprehensive comparisons of model predictions with observations in order to generate probability distribution functions of the differences between modeled and observed values. The current paucity of such appropriate evaluation data sets prompted the workshop recommendation that improvements are needed in emissions, meteorological, and chemical observational data bases. In addition to improved temporal resolution, enhanced spatial resolution of the monitoring data would provide the opportunity to determine the spatial representativeness of point measurements, an issue of importance to the performance evaluation of long-range transport models.

EULERIAN LONG-RANGE TRANSPORT MODELS

Eulerian long-range transport models have been designed to study relationships between source emissions and receptor air quality and deposition over large areas. At present there are several large-scale development activities directed at constructing models of the physical and chemical processes occurring in the atmosphere, and of the effect of these processes on the regional transport and deposition of airborne pollutants.

It was the opinion of most workshop participants that appropriate criteria and procedures for quantifying errors in Eulerian models should be based on the following two considerations: 1) the need to effectively demonstrate the impact of alternative emission control strategies, and 2) the need to quantify indices of model performance over the total domain or over subdomains representative of different meteorological processes. The former could be semi-quantitative (relying on relative signal changes) until our experience with the models permits determination of a more objective numerical criterion. The latter would make use of measures of the models' precision in simulating time and space variations in most model output parameters to guide in the systematic improvement in process representation.

The uncertainty in Eulerian transport model outputs consists of input uncertainty and model formulation uncertainty. The formulation uncertainty will include a component relating to the representation of the physical-chemical processes and partly attributable to the mathematical integrations. Insight into the models' response to arbitrarily varying inputs for a particular formulation can be studied effectively by methods currently available.

Complete evaluation of the Eulerian long-range transport models requires systematic comparison with quality-controlled observational data over as extensive a model domain as possible. It should be recognized that the effect of subgrid-scale processes, turbulence representation in transport processes, and problems of specification of input fields will result in a limit of predictability analagous to that for meteorological forecast models.

Since such large contributions to uncertainty in Eulerian model predictions have been due to limitations of available input data, it is generally felt that model uncertainty can be reduced by increasing the spatial and temporal resolution of the input data. However, since the cost of obtaining higher-density and more frequent measurements may be prohibitive, it is important to estimate how model uncertainty will decrease as the input resolution is increased. One approach to quantifying the improvement is to use existing models to study their sensitivity to input data. It was therefore recommended that direct simulation studies be initiated to quantify the sensitivity of Eulerian model predictions to increases in spatial and temporal resolution of the input data, bearing in mind that, in the absence of prior model testing against reliable data, the derived output sensitivity may partly reflect model artifacts.

LAGRANGIAN LONG-RANGE TRANSPORT MODELS

Lagrangian long-range transport models are now being used widely to diagnose source-receptor relationships for ambient SO_2 concentrations and for sulfur deposition, and to estimate the potential changes in sulfur concentration and deposition values following changes in the emissions distribution of SO_2. In general, the Lagrangian models are popular because: 1) they are simpler in concept than Eulerian models and generally less expensive to operate, and 2) they are presently operational.

On a daily basis, Lagrangian transport models can give some useful information on SO_2 and particulate $SO_4^=$ concentrations, but their strength is in the reproduction of seasonal and annual distributions of daily concentrations rather than in pair-wise agreement. The comparison of daily estimates of SO_2 and $SO_4^=$ with observations does serve the purpose of identifying meteorological regimes during which model performance is improved versus regimes during which it is poor. While the pair-wise agreement between predicted and observed concentrations does not in itself guarantee reliable estimates of the source-receptor relationships, it does give more confidence in defining such relationships when the agreement is high.

There are actually few essential differences between the Lagrangian and Eulerian long-range transport models apart from the frame of reference with which the flow is treated. However, the simplicity of Lagrangian models forces trade-offs that limit their resolution relative to Eulerian models. The specification of nonlinear chemical reactions, for example, is possible in Lagrangian formulations, but the implied horizontal mixing of Lagrangian models limits their resolution of impact from specific source regions. If the Lagrangian models

are reformulated to include all major effects of stratification within air parcels, the advantages associated with their simple and basic formulation are quickly lost and are replaced by less advantageous complexity.

Since one of the principal uses of Lagrangian long-range transport models is the establishment of source-receptor relationships, it becomes necessary to evaluate the ability of the models to reproduce these relationships. Unfortunately, there are few data currently available for this purpose. Presently, the ability of a Lagrangian model to reproduce source-receptor relationships is circumstantial, based on ability to reproduce observed concentration patterns. The workshop participants recommended conducting future field studies 1) to evaluate the ability to reproduce wind trajectories through use of passive, nonreactive tracers, and 2) to evaluate the parameterization of depositions with tracers that emulate the pollutants of interest.

Lagrangian transport models represent reasonable approximations to complex atmospheric processes. The user of model predictions must, however, keep in mind the spatial limitations imposed by the Lagrangian framework in situations of near-field deposition and in the vertical stratification of pollutants. Furthermore, the application of these models with linear chemical transformations to future emission scenarios must also be performed cautiously.

UNCERTAINTY WORKSHOP SUMMARY

In addition to Eulerian and Lagrangian long-range transport models, the workshop participants discussed implications of uncertainty in stochastic models. A long-range transport model is characterized as stochastic when it is based upon models for the probabilities of selected events associated with long-range transport and deposition. Most stochastic models are designed to estimate long-term values of concentration and deposition of pollutants. Such models are empirical in the sense that it may not be possible to provide rigorous justification for all the assumptions on which they are based. Their validity derives primarily from the goodness of fit between model estimates and corresponding observations.

As stated previously, the workshop participants placed the highest priority with regard to the elucidation and quantification of uncertainty in all types of long-range transport models on the development of improved observational data bases for model testing and performance evaluation. These recommendations along with suggestions for determining the uncertainty inherent in model formulations will be detailed in the forthcoming AMS workshop report (American Meteorological Society, 1987).

INTERNATIONAL MODEL EVALUATION

Following the Memorandum of Intent effort and the AMS Uncertainty Workshop, several of the United States and Canadian scientists joined forces to conduct the intercomparison

and evaluation of eleven linear-chemistry statistical and Lagrangian atmospheric transport models of sulfur deposition. This International Sulfur Deposition Model Evaluation (ISDME) was co-sponsored by the Office of Research and Development of the U.S. Environmental Protection Agency and by the Atmospheric Environment Service of Environment Canada. Unlike previous similar model evaluation efforts and in accordance with some of the AMS workshop recommendations, the ISDME effort focused on the ability of the models to replicate the spatial patterns of seasonal as well as annual amounts of sulfur wet deposition within the uncertainties of the currently available monitoring data.

The emphasis on pattern replication is based on the fact that point measurements are not necessarily representative of the area of model predictions due to local spatial variabilities in meteorological conditions and ambient concentrations. And rather than comparing predictions to the best estimates of the observations, the ISDME evaluation determined whether and by how much the predictions were outside uncertainty limits of the interpolated observations. Based on these uncertainty limits, the statistical significance of the predicted/observed differences was determined. A more complete summary of the ISDME model evaluation results is being presented in another paper at this meeting (Voldner et al., 1987).

POLICY PERSPECTIVE

Air quality simulation modeling continues to play a significant role in environmental policy and regulatory decision making. Air quality management, through the implementation of air quality and emission standards, has formed the basis of the Clean Air Act legislation in the United States. This management framework is based on the concept that quantitative links between pollutant emissions and ambient air quality can be developed which provide viable guidance as to the most effective and efficient pollution abatement strategies to meet existing air quality standards, or to consider future policy options for the mitigation of a pending environmental problem (Demerjian, 1985a).

As our understanding of attendant atmospheric processes governing the transport, transformation, and deposition of pollutants evolves, so does our ability to prescribe the predictive accuracy of models that integrate these processes to simulate the fate and transport of pollutants in the atmosphere. But our understanding is incomplete as is our ability to precisely monitor the state of the atmosphere at all times and in all space. As a result, the models must be regarded as imperfect tools providing imperfect predictive information to the user community (Fox, 1984). This fact should not be construed as a condemnation of air quality simulation modeling or as disincentive for their use in air quality management. It is meant rather to convey that the limits on our ability to predict most chemical and physical dynamics of atmospheric systems are real, but are becoming more quantifiable with our *expanding knowledge.*

Uncertainty Implications

In general, transport models are designed to be applied with various emissions reduction scenarios to determine the most effective strategy for attainment of ambient air quality standards. Some of these standards have been based on health effects criteria and must provide an adequate margin of safety to ensure protection of public health, while others are based on the causative effects of airborne pollutants on visibility degradation, water quality deterioration, crop losses, and materials damage. Regardless of intended effects of emissions control, the first point to be addressed is the source of the airborne pollutants, i.e., 1) whether the precursor pollutants are of natural or man-made origin; 2) whether they come from local sources or from distances exceeding hundreds of kilometers; and 3) whether it is possible to define the geographic origin of pollutants that are deposited in a particular downwind region.

Model accuracy is also a critical element in several of the suits and petitions by States to control transported air pollutants under the interstate provisions of the Clean Air Act. The U.S. Environmental Protection Agency has considered available models to be inadequate in their present forms to address the question of long-range pollution transport; consequently, the Agency has historically not assessed the effects of air pollution that travels beyond 50 kilometers. However, initial steps are being taken by the Agency to remedy this situation through various applications of the Regional Oxidant Model (ROM) (Lamb, 1982). Presently these trial applications involve regulatory impact analyses of rural ozone concentrations, site emissions impact of treatment storage disposal facilities, and the Regional Oxidant Modeling of Northeast Transport (ROMNET).

Uncertainties about which pollutants to control, as well as the uncertain relationships between emissions reductions and deposition reductions, complicate the policy objective of reaping the greatest possible benefit from the costs of controlling emissions. Using the current long-range transport models, scientists are attempting to confidently project the precise pattern of deposition reductions that will result from a specified emissions control plan. Until this confidence is achieved, a control program designed and implemented today might not produce the maximum benefits achievable for a given cost.

Role of the Scientist

Uncertainties in the relationships between a causative pollutant and a health or materials damage effect, even if quantifiable, cannot currently be expressed as such under the present law, that is, as a probabilistic rather than a deterministic absolute standard. Therefore, to the extent found possible, such an uncertainty needs to be incorporated within the context of a margin of safety. Thus, the scientists must address the development of quantitative measures as well as the effective utilization and communication of transport model uncertainty in order to better serve the policy and regulatory decision-making communities.

In many instances, the quantification of such scientific uncertainty, or lack thereof, becomes a manipulative factor between contending interests to provide a rationale for positions they advocate. Scientists, to some extent, exascerbate this contention by not maintaining total objectivity in presenting otherwise factual data, but instead allow their value systems to affect their scientific judgement either subtly or intentionally.

In any event, the scientist's role is to provide his best objective and factual judgment on the nature and magnitude of the uncertainty associated with the scientific issues that may have a direct impact on public policy choices. The ramifications of the scientific uncertainty with regard to sorting out what public policy choices should be made is not part of the scientist's judgmental process, but the responsibility of the policy analyst/decision maker.

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